

ARMY RESEARCH LABORATORY



Elastic Behavior of an Atomic Lattice Under Large Volumetric Strains: The Quasi-Harmonic Idealization

by Steven B. Segletes

ARL-TR-1357

May 1997

19970612 056

Approved for public release; distribution is unlimited.

DTIC QUALITY INSPECTED 1

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorized documents.

Citation of manufacturer's or trade names does not constitute an official endorsement or approval of the use thereof.

Destroy this report when it is no longer need. Do not return it to the originator.

Army Research Laboratory

Aberdeen Proving Ground, MD 21005-5066

ARL-TR-1357

May 1997

Elastic Behavior of an Atomic Lattice Under Large Volumetric Strains: The Quasi-Harmonic Idealization

Steven B. Segletes

Weapons and Materials Research Directorate

Abstract

The implications of Segletes' recent equation of state are examined, when idealized to the condition defined as quasi-harmonicity. Results indicate that at large volumetric strains, a proportionality no longer holds, in general, between the volumetric and vibrational stiffnesses. The governing relation between these two stiffnesses is presented and is a function of the characteristic frequency of the lattice, alternately expressed in terms of the lattice spacing. It is further shown that the quasi-harmonic idealization of Segletes' equation will approach the harmonic approximation in the limit.

Acknowledgments

I would like to express a great deal of gratitude to Dr. Michael J. Scheidler, of the U.S. Army Research Laboratory (ARL), for providing an outstanding review of the work and, in so doing, helping to improve the quality of the material presented. I am similarly grateful to Mr. Konrad Frank and Dr. Andrew Dietrich, of ARL, for their constant encouragement and support of the author's efforts on this topic. Finally, eternal thanks goes to my wife, Gabriele, who, through her support and example, encourages excellence in others.

INTENTIONALLY LEFT BLANK.

Table of Contents

	<u>Page</u>
Acknowledgments	iii
List of Figures	vii
1. Background	1
2. Segletes' Equation of State and the Quasi-Harmonic Idealization	9
3. Force-Based Moduli	11
4. The Relationship Between the Volumetric and Vibrational Moduli	12
5. Conclusions	19
6. References	23
Distribution List	27
Report Documentation Page	45

INTENTIONALLY LEFT BLANK.

List of Figures

	<u>Figure</u>		<u>Page</u>
1.	Relative values of the vibrational ($\partial F_{\text{vib}}/\partial x$) and volumetric ($dF/d\lambda$) stiffnesses, as a function of the relative characteristic temperature (or frequency), for a material obeying the quasi-harmonic idealization		21
2.	Ratio of volumetric to vibrational (force-based) moduli, as a function of the relative characteristic temperature (or frequency), for a material obeying the quasi-harmonic idealization		21
3.	Ratio of volumetric to vibrational (force-based) moduli, as a function of relative volume, for a material obeying the quasi-harmonic idealization		22
4.	Relative cold compression energy versus relative lattice spacing, with reference Grüneisen value, Γ_0 , as a parameter, for quasi-harmonic material		22

INTENTIONALLY LEFT BLANK.

1. Background

The harmonic approximation has been the traditional method to analyze atomic vibrations and lattice behavior, dating back to Planck. Several years later, in the early 1900s, Einstein, Debye, and Born and von Karman [1] used the approximation to develop theories of lattice specific heat. In the years that followed, Brillouin [2] also employed the harmonic approximation to analyze wave propagation in lattice structures.

In the harmonic approximation, atoms vibrate with sinusoidal motion. In order for an atom within the crystal lattice to retain this harmonic behavior, the specific potential energy well of the lattice, $E_{pot}(r)$, must be parabolic in shape, where r is the coordinate of the atom in question within the lattice. Specifically, $\Delta E_{pot} \sim (r - r_0)^2$. Under these conditions, the restoring force to the atom is proportional to its displacement from the rest position, and the resulting oscillatory motion of the atom is sinusoidal—that is to say, harmonic. The harmonic motion of an atom has a single frequency associated with it, ω_0 , and that frequency is calculable, just as in macroscopic vibration theory, by the relation $\omega_0^2 = (-\partial P / \partial r) / M$, where M is the mass of the atom, P is the restoring force, and $-\partial P / \partial r$ is the local spring constant in the direction of the disturbance, which, for the harmonic case, is independent of position. If a lattice of vibrating atoms is considered, rather than just a single oscillating atom, a whole spectrum of frequencies is shown to arise in the lattice. Furthermore, in a three-dimensional (3-D) lattice, for every frequency of the spectrum associated with a disturbance in the direction of the wave propagation (a longitudinal wave), there are two vibrational components associated with disturbances perpendicular to the direction of wave propagation (shear waves).

Let us remember, now and throughout this report, that vibrations are the means by which internal (*i.e.*, potential) and kinetic energy are exchanged in a spring. Every type of vibration, no matter how complicated kinematically, has an associated spring constant (or alternately, wave speed) and displacement variable. The derivative of the spring's potential energy with respect to the displacement variable is known as the "force," and the derivative of the force with respect to this displacement variable is the local spring constant (or stiffness), which governs the vibrational frequency for infinitesimal vibrations of the spring.

An early, important result of lattice-vibration theory was in showing that vibrational energy in a lattice can manifest itself as thermal pressure only if the lattice vibrational frequencies change with lattice deformation—that is to say, if the potential energy well is not parabolic in shape. This condition of nonparabolicity is referred to as anharmonicity. Likewise, nonparabolic terms in a Taylor expansion of the potential energy well about the reference lattice spacing are called anharmonic terms. In practical terms, the empirical metric for anharmonicity usually entails measuring the nonparabolicity of the lattice's energy well only at the reference lattice spacing (*e.g.*, the method used by Rose *et al.* [3]). Here and throughout this report, the reference condition is one of zero temperature and pressure.

Quantitatively, a lattice's vibrational energy gets coupled into thermal pressure by way of the Grüneisen function, macroscopically defined as $\Gamma = V(\partial p / \partial E)_v$, where V is the material's specific volume, and p and E are the pressure and specific energy of the material, respectively. From lattice theory, there is a Grüneisen value associated with each vibrational frequency in the lattice, given by the following expression and taken at constant temperature, T :

$$\Gamma_i = - \frac{V}{\omega_i} \left(\frac{\partial \omega_i}{\partial V} \right)_T, \quad (1)$$

where Γ_i is the Grüneisen value associated with the frequency, ω_i , of a longitudinal or transverse (*i.e.*, shear) vibration. Were the Γ_i values for each frequency truly independent of each other, the macroscopically observed Γ value, being an aggregate of all the Γ_i , would be very difficult to characterize in terms of the individual Γ_i . However, one fortunate simplification to the problem arises from Grüneisen's assumption, which was originally made based on empirical data and later supported theoretically by the lattice theory of Debye. The assumption asserts that the whole spectrum of lattice vibrational frequencies changes in a characteristically similar fashion with lattice spacing, so that the knowledge of how one characteristic frequency changes with volume defines the behavior of the complete vibrational spectrum. The effect on eqn (1) is to remove the '*i*' subscript, with the resulting equation being characteristic of the behavior of the complete vibrational spectrum. From the early theories of specific heats, this characteristic frequency (a

microscopic quantity) was shown to be directly proportional to a characteristic temperature, Θ (a macroscopic quantity). Thus, it is common to find, in the literature, an interchangeable use of the expressions (ω/ω_0) and (Θ/Θ_0) , where the "0" subscript refers to the reference value. Another simplification is afforded by the approximation, supported by data, that, for solids in the absence of phase change, eqn (1) is independent of temperature, so that the partial derivatives in eqn (1) become ordinary. In this case, Γ , ω , and Θ all become functions of specific volume only. Work in the area of a temperature-dependent Grüneisen function was done by both Blackman [4] and Barron [5], who examined and modeled the variation of Γ with temperature at low values of temperature ($T/\Theta \ll 1$) and found mild variations. Later, Grodzka [6] summarized work, using the compression of porous media, which indicated that some materials (notably aluminum) seem to have a significant decrease in Γ at elevated temperatures. Aluminum aside, the temperature independence of the Grüneisen parameter, while empirical, seems valid over a wide range of conditions and solids.

Even with the simplifications afforded by the temperature-independent, coupled frequency form of eqn (1), the difficulty still arises of how to describe the anharmonic behavior of lattices, given that the prevailing theories describing their fundamental behavior are based on harmonic approximations. Slater [7] and later Dugdale and MacDonald [8] used the harmonic approximation as a basis to develop anharmonic theories of the Grüneisen function.

To better understand the model of Dugdale and MacDonald [8], as well as more recent work, let us construct a framework for analyzing anharmonic vibrations. Given a simple spring-mass system, consider replacing the linear (harmonic) reference spring with a nonlinear (*i.e.*, anharmonic) spring. Vibration theory may be used to compare the frequencies of vibration for these two systems. Though the frequency of vibration for a nonlinear spring changes with amplitude, the situation of low-temperature atomic vibrations may be likened to the situation of a spring experiencing infinitesimal vibrational amplitudes superimposed about a nominal spring extension. In fact, the notion of thermal expansion in a solid is directly analogous to a nonlinear spring, in that, as the temperature is raised, the vibrational amplitude increases, and as the amplitude increases, the nonlinearity of the spring causes the average spring extension (*i.e.*, density) to change, even though the nominal applied force remains constant. The nominal spring extension is analogous, in a lattice, to the atomic spacing relative to the reference

configuration, and the small vibrational oscillations that occur do so about this deformed configuration. Under this condition of infinitesimal vibrations, corresponding to the low-temperature condition of the lattice, the vibrational frequency of a nonlinear spring is obtainable by way of perturbation theory (*i.e.*, by linearizing the problem and considering small perturbations in displacement about the nominal extension). For a given mass, the local spring stiffness determines the vibrational frequency of the spring and is given by the local slope of the force-displacement curve for the spring, which is a function only of the current spring extension. Thus, the relationship that governs how the frequency response is altered by substituting the anharmonic spring for the harmonic reference spring is given as

$$\frac{\omega^2}{\partial F/\partial x} = \frac{\omega_{ref}^2}{\partial F_{ref}/\partial x} = -\frac{1}{M} , \quad (2)$$

where the “*ref*” subscript refers to the reference, harmonic spring.

To further extend the spring analogy to a lattice of atoms, consider the case of a 3-D lattice of spring-connected identical masses. In the general case, the lattice may support physical motion both in the direction of, as well as transverse to, the direction of wave propagation. Furthermore, to be general, we allow the lattice/spring topology to include diagonally connected masses, such that a displacement in one direction may induce force and/or motion in the perpendicular directions. In this general case, the vibrational frequency spectrum of the spring-connected lattice includes components due to both longitudinal and transverse vibrations. Such a frequency spectrum, aggregated of both the longitudinal and transverse spectra, is directly analogous to that found in actual solids. Brillouin [2] has shown that, if a Debye frequency spectrum is assumed for a material, the aggregated characteristic temperature (frequency) is describable as a composite of the longitudinal and transverse frequency spectra as follows:

$$\frac{1}{\Theta_l^3} + \frac{2}{\Theta_t^3} = \frac{3}{\Theta^3} . \quad (3)$$

Others [9, 10] have accomplished a similar result by relating an aggregate of longitudinal and transverse wave-propagation velocities (related to their associated frequency, ω , and wavelength, λ , via $C = \omega\lambda$) directly to the Grüneisen function (related to the frequency spectrum by eqn [1]). For example, Pastine [9] provided this relation as

$$\Gamma = 1/3 [1/3 - (V/C_l) dC_l/dV] + 2/3 [1/3 - (V/C_t) dC_t/dV] , \quad (4)$$

where C_l and C_t refer to the longitudinal and transverse wave speeds, respectively. By relating these component wave speeds to variations in the Poisson ratio, Pastine was able to derive a Grüneisen expression as a function of Poisson's ratio and showed, for the special case of a monatomic face-centered cubic crystal, a result quite close to the theoretically derived result of Barron [5]. However, for the general case, no guidance was offered on appropriate selection of functional forms. Vashchenko and Zubarev [10] adopted a similar approach, but assumed a particular fitting form for the Poisson ratio, in terms of the cold pressure curve and a fitting parameter.

Unlike these other approaches, Plendl [11] considered the measured frequency spectra for real materials, as opposed to using idealized relationships like eqns (3) and (4). Rather than attempting a decomposition of the spectrum into longitudinal and transverse components, he was able to bypass such an approach and show that the characteristic frequency of a material is that frequency at the center of gravity of the frequency spectrum, $f(\omega)$, the so-called "centro-frequency," which is given by

$$\omega_{ctr} = \frac{\int_{\omega_1}^{\omega_2} \omega f(\omega) d\omega}{\int_{\omega_1}^{\omega_2} f(\omega) d\omega} , \quad (5)$$

where the frequency range of integration is selected to comprise the entire range of the acoustical vibration spectrum.

The current analysis follows the lead of Plendl, in that no explicit decomposition of the vibrational spectrum into longitudinal and transverse components will be performed. The mere fact that a characteristic frequency may be aggregated, in some manner, from the longitudinal and transverse frequency spectra (by way of eqn [3], [4], [5], or otherwise) allows us to introduce the concept of a vibrational spring constant, $\partial F_{vib}/\partial x$, which is, by definition, the spring constant that characterizes the aggregated (longitudinal plus transverse) vibrational frequency spectrum. If a lattice had no diagonal coupling and didn't support transverse (shear) waves, the characteristic vibrational stiffness would simply reduce to the stiffness of the component longitudinal spring. The vibrational spring constant will, like the stiffness of a nonlinear spring, be a function of the nominal lattice spacing. By way of this construct of the vibrational spring constant, eqn (2) may be generalized to case of a 3-D coupled lattice:

$$\frac{\omega^2}{\partial F_{vib}/\partial x} = \frac{\omega_{ref}^2}{\partial F_{ref}/\partial x} , \quad (6)$$

where, now, ω is a characteristic frequency of the vibrational spectrum, rather than the specific frequency of the component spring.

Let us analyze a lattice where the specific unit lattice spacings (*i.e.*, length per cube-root unit mass) along the principal lattice directions, x , y , and z , are expressed in terms of the specific volume of the unit cell as $V = \lambda^3 = xyz$, where λ is an averaged unit lattice spacing per cube-root unit mass. For the case of zero-temperature volumetric compression or distention, a specific force may be defined as that force (per 2/3 power unit mass) acting on the face of a unit cell of the lattice, given as $F = p_c \lambda^2 = p_c V^{2/3}$. In this definition, p_c is the cold (0° isotherm) pressure and, thus, the force is positive in compression.

If nothing else were known of the vibrational frequency spectrum, it would be natural to investigate the proportionality of $\partial F_{vib}/\partial x$ and $dF/d\lambda$, since, for a one-dimensional (1-D) harmonic

lattice, these two quantities would, in fact, be identically equal. The assumption that the characteristic vibrational stiffness of a 3-D spring can be made proportional to an associated volumetric stiffness has been pervasive throughout the literature. When Debye theory indicated that the characteristic frequency varied as an aggregate of the elastic wave speeds, Slater [7] assumed a constant Poisson ratio and related the aggregated vibrational stiffness (in terms of wave speeds) directly to volumetric compressibility (although Slater actually concluded something closer to [but not quite] $\omega^2 \sim -dp/d\lambda$ rather than $-dF/d\lambda$). Brillouin [2] derives results utilizing $\omega^2 \sim d^2E_c/d\lambda^2$, the right-hand side being merely $-dF/d\lambda$. It will be shown that Dugdale and MacDonald [8] also utilized this proportionality. More recently, Guinea *et al.* [12] explicitly assumed this proportionality when trying to infer a relationship between the universal cold curve and the Grüneisen function.

The effect of such an assumption of proportionality on eqn (6) is that a $dF/d\lambda$ term may be substituted for each $\partial F/\partial x$. With this substitution, the derivatives with respect to λ are convertible to volume derivatives through the chain rule,

$$dF/d\lambda = dF/dV \cdot dV/d\lambda = (p_c V^{2/3})' \cdot 3V^{2/3} , \quad (7)$$

where the prime symbol (') denotes ordinary differentiation with respect to specific volume. With this substitution, eqn (6) becomes

$$\frac{\omega^2}{(p_c V^{2/3})'} = \frac{\omega_{ref}^2}{(p_{ref} V^{2/3})'} . \quad (8)$$

If one takes the volume derivative of eqn (8) and divides the result by eqn (8) itself, one obtains

$$2 \frac{d\omega/dV}{\omega} - \frac{(p_c V^{2/3})''}{(p_c V^{2/3})'} = 2 \frac{d\omega_{ref}/dV}{\omega_{ref}} - \frac{(p_{ref} V^{2/3})''}{(p_{ref} V^{2/3})'} . \quad (9)$$

The first term from each side of the equation is related to the Grüneisen function and may be substituted, using the temperature-independent, characteristic-frequency form of eqn (1), to obtain

$$2 \frac{\Gamma}{V} = -\frac{(p_c V^{2/3})''}{(p_c V^{2/3})'} + 2 \frac{\Gamma_{ref}}{V} + \frac{(p_{ref} V^{2/3})''}{(p_{ref} V^{2/3})'} . \quad (10)$$

At this point, the values for the harmonic, reference spring may be substituted. As already mentioned, the value for Γ in a harmonic system is identically zero, since ω is constant, and the last term involving the pressure behavior of the reference system may be acquired using the definition $p_{ref} = -dE_{ref}/dV$, where E_{ref} is the parabolic energy well expressed in terms of V rather than x . The result is the well-known Dugdale-MacDonald relation:

$$\Gamma = -\frac{1}{3} - \frac{V}{2} \frac{(p_c V^{2/3})''}{(p_c V^{2/3})'} . \quad (11)$$

Inserting the harmonic energy potential into this equation results in a Grüneisen value of zero. Such a result illustrates the criticism, by Dugdale and MacDonald [8], of the model of Slater [7]—namely, that inserting the harmonic cold curve into Slater's model does not produce the required value of $\Gamma = 0$.

This report will show, on the basis of Segletes' recently proposed equation of state, that, for a 3-D lattice, the presumed proportionality between the volumetric and vibrational stiffness, which has pervaded the literature and leads to the model of Dugdale and MacDonald, is strictly true only in the harmonic limit of approximation. Force-based, vibrational and volumetric moduli will be compared, for the idealized case of quasi-harmonicity (defined in the next section), with the more general case to be addressed in a subsequent report. Finally, the quasi-harmonic idealization of Segletes' equation of state will be shown to approach the harmonic approximation as the Grüneisen function approaches zero in the limit.

2. Segletes' Equation of State and the Quasi-Harmonic Idealization

Recently, Segletes [13, 14] proposed an equation of state, of Grüneisen form, that properly captures both the lattice-potential and thermal pressure behavior for a variety of crystalline materials, into the megabar range of pressures. The model was inspired by the universal cold curve of Rose *et al.* [3]. However, unlike the model of Rose and other recent equation-of-state models, (*e.g.*, Vinet *et al.* [15, 16]; Baonza, Cáceres, and Núñez [17]; and Baonza *et al.* [18]), the model of Segletes casts the lattice energy potential in terms of the characteristic temperature of the lattice (*i.e.*, the lattice vibrational frequency), rather than lattice spacing (density). The equation of state is given as

$$p\psi - E = E_b \left\{ \left[(\Theta/\Theta_0)^K - 1 \right] + K(K-1) (\Theta/\Theta_0)^K \ln(\Theta/\Theta_0) \right\} . \quad (12)$$

In this equation, p and E are the pressure and specific internal energy respectively, K is a parameter, given by $C_0/(\Gamma_0\sqrt{E_b})$, where C_0 is the reference bulk sound speed at zero temperature and pressure, E_b is the specific lattice binding energy, and $\psi = V/\Gamma = (\partial E/\partial p)_v$ is a thermodynamic variable introduced by Segletes [19, 20] for ease in manipulating the governing equations. In terms of this variable, ψ , the temperature-independent, coupled-frequency form of eqn (1) is given as

$$\frac{\Theta'}{\Theta} = -\frac{1}{\psi} , \quad (13)$$

where the proportionality between Θ and ω has been utilized. The generalized cold curve associated with eqn (12) is

$$E_c = E_b \{ 1 - (\Theta/\Theta_0)^K [1 - K \ln(\Theta/\Theta_0)] \} \quad (14)$$

and

$$p_c = \frac{E_b K^2}{\psi} (\Theta/\Theta_0)^K \ln(\Theta/\Theta_0) . \quad (15)$$

When the K parameter takes on a value identically equal to unity and the Grüneisen function varies as $\Gamma \sim V^{1/3}$ (i.e., $\Gamma \sim \lambda$), the equation takes on behavior that will hereafter be called quasi-harmonic. If we denote the variables of the quasi-harmonic equation of state as hatted quantities ($\hat{}$), the quasi-harmonic cold curve becomes

$$\hat{E}_c = \hat{E}_b \{1 - (\hat{\Theta}/\hat{\Theta}_0) [1 - \ln(\hat{\Theta}/\hat{\Theta}_0)]\} \quad (16)$$

with the Grüneisen requirement translating to

$$\hat{\psi} \sim V^{2/3} . \quad (17)$$

Eqns (16) and (17) are interpreted as quasi-harmonic for a number of reasons. It is immediately obvious that, when K equals unity, many terms drop out from the general equation of state, eqn (12), and the equations become greatly simplified. Furthermore, Segletes and Walters [21, 22] examined the equation of state using a simple power law, V^x , to model the ψ function. They noted that, over a wide range of anharmonicity, the exponent, x , required to fit well the model of Rose *et al.* [3], varied linearly with Rose's anharmonicity parameter, η . Though it did not match precisely in the limit, an exponential relation of $\psi \sim V^{2/3}$ was the limiting trend for the case where Rose's anharmonicity, η , approached zero. Segletes and Walters also showed, for the case of $K=1$ and $\hat{\psi} \sim V^{2/3}$ (the quasi-harmonic case), that the Segletes equation of state satisfies the relation

$$(p_c V^{2/3}) + [2 + 2/3 (\hat{\psi}/V)] \hat{\psi} (p_c V^{2/3})' + \hat{\psi}^2 (p_c V^{2/3})'' = 0 , \quad (18)$$

whereas the Dugdale-MacDonald relation, eqn (11), noted for its harmonic limiting behavior,

satisfies

$$\left[2 + \frac{2}{3} (\psi/V)\right] \psi (p_c V^{2/3})' + \psi^2 (p_c V^{2/3})'' = 0 \quad . \quad (19)$$

Eqns (18) and (19) differ by only the first term of eqn (18).

In a subsequent report, Segletes will treat the more general form of his equation of state, by showing that the K parameter in eqns (12), (14), and (15) must, for real materials, be a (slowly varying) function of volume, which asymptotes to the quasi-harmonic case in the large-volume limit. In the meantime, the cause of the disparity between the idealized form of Segletes' model and that of Dugdale and MacDonald [8] will be shown to arise from the fact that, for large volumetric strains, the volumetric and vibrational stiffnesses, $dF/d\lambda$ and $\partial F_{vib}/\partial x$, respectively, are not proportional.

3. Force-Based Moduli

The interactions within a lattice are governed by forces acting over distances. On this basis alone, force and distance would seem to be the natural variables governing the interactions within a lattice. More compelling, however, is the fact that Segletes' equation of state shows a very distinct preference for being analyzed in a force-based framework. Eqn (18) is just one example of how, time and again, the term grouping $(p_c V^{2/3})$, which is the force on the face of the lattice unit cell (per $2/3$ power unit mass), appears. It is for this reason that subsequent results will be analyzed in a force-based framework, by which it is meant that moduli will be expressed in terms of force gradients, rather than stress gradients. To this end, force-based moduli will be defined for a zero-temperature lattice, at an arbitrary volumetric compression or distention, under the influence of an infinitesimal, superimposed, elastic disturbance.

In a force-based frame, a modulus, with units of stress, may be associated with a given spring constant. From considerations of dimensional analysis, the modulus should be of the form spring constant divided by characteristic length. Alternately, a force-based modulus, associated with the volumetric spring constant, $dF/d\lambda$, for example, may be defined by starting with the stress-based

modulus definition (*i.e.*, bulk modulus), substituting a force term for the stress (pressure) term, and dividing the result by the specific area (*i.e.*, area per $2/3$ power mass) over which the force is acting. For a lattice that is only deformed volumetrically, this area is λ^2 , the specific volume to the $2/3$ power. Thus,

$$B_F = -\frac{1}{\lambda^2} \frac{dF}{dV/V} = -V^{1/3} \frac{d(p_c V^{2/3})}{dV} = -\frac{1}{3\lambda} \frac{dF}{d\lambda} . \quad (20)$$

Comparison of the stress-based bulk modulus, B , and the force-based one in eqn (20) reveals that, in general, $B_F = B - 2p_c/3$. Under conditions where the pressure and temperature are zero, the force-based volumetric modulus will equal the stress-based bulk modulus in value.

Turning now to the vibrational spring constant, $\partial F_{vib}/\partial x$, an associated force-based modulus, call it J_F , may be defined. As in the case of the vibrational spring constant itself, this modulus implicitly includes the effects of both longitudinal and shear waves. For a cubic lattice, it is given, in terms of λ , by

$$J_F = -\left(\frac{1}{yz} \frac{\partial F_{vib}}{\partial x/x} \right)_{x=y=z=\lambda} = -\frac{1}{\lambda} \frac{\partial F_{vib}}{\partial x} . \quad (21)$$

4. The Relation Between the Volumetric and Vibrational Moduli

We will summarize what is known of the problem at hand by enumerating a list of statements already discussed, so that subsequent reference may conveniently be made to the ideas contained in the following statements:

(1) In a Grüneisen material:

(a) the vibrational spectrum of a lattice is composed of longitudinal and transverse (shear)

vibrational components. This spectrum may be characterized either in terms of characteristic wave speeds or by a characteristic frequency;

- (b) the characteristic frequency of the vibrational spectrum varies with volume in the same manner as the characteristic temperature, $\omega \sim \Theta$; and
 - (c) the characteristic temperature, Θ , is related to the ψ function (and thus Γ) by way of eqn (13).
- (2) The characteristic frequency, ω , of the vibrational spectrum of a lattice may be directly related to an associated spring constant, designated $\partial F_{vib}/\partial x$, of a material, such that the characteristic frequency varies as $\omega^2 \sim \partial F_{vib}/\partial x$. This spring constant may be alternately expressed as a vibrational modulus, designated J_F , and defined in eqn (21).
- (3) The volumetric stiffness, $dF/d\lambda$, is directly derivable from a material's equation of state, and may be alternately expressed in terms of a volumetric modulus, B_F , defined in eqn (20).
- (4) Segletes' equation of state, which fits the behavior of crystalline solids very well, expresses the behavior of the lattice in terms of relative characteristic temperature, Θ/Θ_0 . Since the characteristic temperature (frequency) function is governed by the vibrational stiffness, $\partial F_{vib}/\partial x$, this equation of state may be used to compare directly the volumetric and vibrational stiffnesses.
- (5) Segletes' model, eqn (12), may be idealized to an important special case, termed the quasi-harmonic idealization, which is characterized by:

- (a) a value of the parameter, K , equal to unity; and
- (b) a ψ function that varies as $V^{2/3}$.

From the cold-pressure curve of Segletes' equation of state, eqn (15), derivatives may be taken, to show that

$$(p_c V^{2/3})' = - \frac{E_b K^2 V^{2/3}}{\psi^2} (\Theta/\Theta_0)^K \left\{ [K + \psi' - 2/3(\psi/V)] \ln(\Theta/\Theta_0) + 1 \right\} . \quad (22)$$

For the quasi-harmonic idealization, defined by statements 5a and 5b, eqn (22) reduces to

$$(p_c V^{2/3})' = - \frac{\hat{E}_b V^{2/3}}{\hat{\psi}^2} (\hat{\Theta}/\hat{\Theta}_0) \left\{ \ln(\hat{\Theta}/\hat{\Theta}_0) + 1 \right\} . \quad (23)$$

If the $\hat{\psi}$ function is quantified as $\hat{\psi} = (V_0^{1/3}/\hat{\Gamma}_0) V^{2/3}$, in accordance with the definition of ψ and statement 5b, then the $dF/d\lambda$ function is given as

$$dF/d\lambda = 3 V^{2/3} (p_c V^{2/3})' = - \frac{3 \hat{E}_b \hat{\Gamma}_0^2}{V_0^{2/3}} (\hat{\Theta}/\hat{\Theta}_0) \left\{ \ln(\hat{\Theta}/\hat{\Theta}_0) + 1 \right\} . \quad (24)$$

We see here why the quasi-harmonic case is an important one—namely, because the interatomic force and its spacial derivatives vary only with the characteristic frequency and not explicitly as a function of lattice spacing (λ or V). The relative ratios of the zero-temperature vibrational and volumetric stiffnesses may be compared as a function of characteristic temperature ratio and are displayed in Figure 1. The upper curve, for vibrations, is parabolic since (according to statements 1b and 2) it is the spring constant which governs the characteristic frequency (and thus characteristic temperature). The lower curve, derived from Segletes' model for the quasi-harmonic case, relates the relative volumetric stiffness to the characteristic temperature. Were these two curves to overlay, the model of Dugdale and MacDonald [8] would prevail. As it is, the vibrational and volumetric stiffnesses for a quasi-harmonic, 3-D lattice do not remain proportional, though they do so approximately near the reference density.

Eqn (24) expresses the volumetric stiffness in terms of the quasi-harmonic, characteristic temperature of the lattice. A converse relationship may be obtained by starting with eqn (18), and making the substitution in the bracketed term that, for the quasi-harmonic case,

$\hat{\Psi}' = 2/3 (\hat{\Psi}/V)$. Employing the fact that $F = p_c V^{2/3}$, the resulting equation may be rearranged to give

$$-\frac{1}{\hat{\Psi}} = \frac{(\hat{\Psi}F'' + (1 + \hat{\Psi}')F')}{(\hat{\Psi}F' + F)} . \quad (25)$$

The left side of the equation is, by way of eqn (13), $\hat{\Theta}'/\hat{\Theta}$. Similarly, the numerator of the right side of the equation is also the volume derivative of the denominator. Thus, we see that

$$\hat{\Theta} \sim \hat{\Psi}F' + F = \frac{\lambda_0}{3\hat{\Gamma}_0} \frac{dF}{d\lambda} + F , \quad (26)$$

which expresses the characteristic frequency in terms of the lattice cell force and its spacial derivative.

To put the comparison in yet another perspective, in terms of the moduli, we compute, from eqns (20) and (24), that $\hat{B}_F/\hat{B}_{0F} = (\lambda_0/\lambda)(\hat{\Theta}/\hat{\Theta}_0)[\ln(\hat{\Theta}/\hat{\Theta}_0)+1]$. Likewise, from eqn (21) and statements 1b and 2, we know that $\hat{J}_F/\hat{J}_{0F} = (\lambda_0/\lambda)(\hat{\Theta}/\hat{\Theta}_0)^2$. We will assume now the initial condition, that $\hat{J}_{0F} = \hat{B}_{0F}$. This assumption corresponds, for a 3-D lattice, to the situation where $(dF/d\lambda)_{V_0}$ equals $3(\partial F_{vib}/\partial x)_{V_0}$. If this assumption should subsequently prove wrong, the sole effect will be that eqns (27) and (30), to follow, will be off by a constant multiplier. The force-based volumetric and vibrational moduli, for the quasi-harmonic case, may thus be directly related as

$$\hat{B}_F/\hat{J}_F = \frac{[\ln(\hat{\Theta}/\hat{\Theta}_0) + 1]}{(\hat{\Theta}/\hat{\Theta}_0)} . \quad (27)$$

A graph of this function is shown in Figure 2, as a function of the quasi-harmonic, relative characteristic temperature, $\hat{\Theta}/\hat{\Theta}_0$. This figure indicates the functional relationship between the force-based volumetric and vibrational moduli for the quasi-harmonic case.

Alternately, this relationship may be expressed as a function of specific volume ratio, by converting characteristic temperature to specific volume. By starting with the quasi-harmonic ψ function, given by

$$\psi = (V_0^{1/3}/\hat{\Gamma}_0) V^{2/3} , \quad (28)$$

one may integrate according to eqn (13) to ascertain the logarithm of the quasi-harmonic frequency function:

$$\ln(\hat{\Theta}/\hat{\Theta}_0) = 3 \hat{\Gamma}_0 [1 - (V/V_0)^{1/3}] . \quad (29)$$

Interestingly, the quasi-harmonic eqn (29) is proportional to the negative of the a^* parameter employed by Rose *et al.* [3], as the nondimensional lattice parameter in their universal cold curve. The model of Rose *et al.*, which was the inspiration for Segletes' equation of state [13, 14], expresses cold energy in terms of compression and is seen from eqn (29) to relate closely to the quasi-harmonic case idealized from Segletes' model. However, unlike Segletes' equation of state, Rose's model does not include thermal pressure effects required for a complete equation of state and has no provisions for Segletes' general case, which is not quasi-harmonic.

Exponentiation of eqn (29) provides the characteristic temperature ratio. The quasi-harmonic characteristic temperature ratio tells exactly why the real world is not quasi-harmonic—because, in the quasi-harmonic case, there is a maximum limiting frequency ratio at vanishingly small volumes, given by $(\hat{\Theta}_{\max}/\hat{\Theta}_0) = \exp(3\hat{\Gamma}_0)$. Such a frequency limit would translate into a cold-compression energy limit, as well. According to various high-compression theories that include electronic effects, finite cold-compression energies under infinite compression do not occur in actual materials. Such limiting compressive behavior, though absent in actual materials,

characterizes both the model of Rose *et al.* [3], as well as the quasi-harmonic idealization. A subsequent report will address how actual materials may be described by Segletes' theory, by departing from the tenets of the quasi-harmonic idealization. In the report to appear, the author intends to show that the data support the notion that, as lattice spacing increases, the behavior of all lattices approaches the quasi-harmonic idealization, and that a departure from this ideal occurs as the lattice spacing becomes small enough to permit interatomic repulsive interactions.

Substitution may be made into eqn (27), in order to express the volumetric to vibrational modulus ratio, in terms of specific volume, as

$$\hat{B}_F/\hat{J}_F = \frac{\{1 + 3 \hat{\Gamma}_0 [1 - (V/V_0)^{1/3}]\}}{\exp\{3 \hat{\Gamma}_0 [1 - (V/V_0)^{1/3}]\}} \quad (30)$$

This relationship is depicted in Figure 3 with the reference, quasi-harmonic Grüneisen parameter value, $\hat{\Gamma}_0$, as a parameter. The figure shows that, only as $\hat{\Gamma}_0$ is made to approach zero, does the quasi-harmonic, zero-temperature, volumetric to vibrational modulus ratio approach a constant value (of unity). The quasi-harmonic lattice force, $F = (p_c V^{2/3})$, may also be expressed in terms of lattice spacing, rather than frequency, through the use of eqns (15) and (29) and the definition that $\lambda = V^{1/3}$:

$$F = \hat{E}_b (\hat{\Gamma}_0/\lambda_0) \exp[3 (\hat{\Gamma}_0/\lambda_0) (\lambda_0 - \lambda)] [3 (\hat{\Gamma}_0/\lambda_0) (\lambda_0 - \lambda)] \quad (31)$$

It is also revealing to study the quasi-harmonic, cold-energy curve, not as a function of frequency, as given in eqn (16), but likewise in terms of relative lattice spacing, using eqn (29) and the relation between λ and V . Figure 4 plots this relation with the reference quasi-harmonic Grüneisen parameter, $\hat{\Gamma}_0$, as a parameter. The energy has been normalized by its limiting ($V = 0$) cold-compression energy, which is finite for the quasi-harmonic case, but will not be so for real materials. The figure clearly shows that, as the reference Grüneisen parameter approaches zero, the quasi-harmonic idealization of Segletes' equation approaches the harmonic case, consistent

with Dugdale and MacDonald [8] theory, as already shown for $\Gamma = 0$. Kittel [23] indicates that, according to harmonic theory, there is no thermal expansion, and the elastic constants are independent of pressure (and temperature). A zero Grüneisen function follows from a zero thermal-expansion coefficient. Thus, the constant ratio of the elastic moduli in Figure 3, for the limiting case of $\hat{\Gamma}_0 = 0$, is further evidence of compatibility with harmonic theory. Furthermore, $\partial F_{\text{vib}}/\partial x$ and $dF/d\lambda$ are proportional for only this limiting case and this proportionality is exactly what would occur for a 3-D lattice of atomic masses connected by simple linear springs. In short, the quasi-harmonic idealization approaches the harmonic limit as $\hat{\Gamma}$ approaches zero.

The harmonic condition has been traditionally expressed by stipulating the potential energy well to be parabolic,

$$\frac{d^3 E_{\text{pot}}}{d\lambda^3} = 0 \quad , \quad (32)$$

thus resulting in a constant characteristic frequency and an identically zero Grüneisen function. We see now that the harmonic approximation is merely the limiting case of the quasi-harmonic idealization of Segletes' equation of state, when the value of the Grüneisen function is made to approach zero in the limit. The quasi-harmonic potential, given by eqn (16), satisfies the following relation:

$$\frac{d^2}{d\lambda^2} \left(\frac{\hat{E}_{\text{pot}}}{\hat{\Theta}} \right) = 0 \quad , \quad (33)$$

where E_{pot} , the potential energy well of the lattice, is the lattice cold energy relative to the infinite lattice separation condition, or $E_{\text{pot}} = E_c - E_b$.

5. Conclusions

The historical use of the harmonic approximation in the study of lattice dynamics has been briefly reviewed to include the development of the Dugdale-MacDonald model of anharmonic lattice behavior. It is shown how, in the case of the model of Dugdale and MacDonald [8], results rely on a certain assumption about the governing elasticity—an assumption that follows from 1-D theory wherein the vibrational and volumetric stiffnesses are proportional. This assumption has been widely adopted by prior treatments of the subject, but has been shown to be inadequate to describe the behavior of a 3-D lattice at large volumetric strain, perhaps as a result of lateral (Poisson ratio) coupling, transverse (shear) waves and/or the presence of non-nearest neighbor interatomic interactions.

The relationship between vibrational and volumetric moduli has been studied using the quasi-harmonic idealization of Segletes' equation of state. The quasi-harmonic idealization is one in which the form of Segletes' equation of state is greatly simplified, while the Grüneisen function takes on a specified, idealized, functional behavior. In the quasi-harmonic idealization, the interatomic force and its spacial derivatives vary only with the characteristic frequency of the lattice and not explicitly with the lattice spacing.

Results indicate that the relationship between the vibrational and volumetric moduli (and their associated natural frequencies) are of different form. In the vibrational case, the stiffness, according to vibration theory, goes as ω^2 , whereas for volumetric distortions of a 3-D lattice, it may be inferred from the idealized form of Segletes' equation of state that the volumetric stiffness goes as $\omega[1 + \ln(\omega/\omega_0)]$. It is this disparity that causes the primary difference between the model of Segletes and previous work by Dugdale and MacDonald [8].

The idealized Grüneisen relationship that governs quasi-harmonic behavior is such that a quasi-harmonic lattice reaches a limiting cold-compression energy (and associated vibrational frequency) in the limit of vanishingly small volume. Such idealized behavior, though not indicative of real materials, is compatible with the theory of harmonic lattice vibrations. This

report explicitly shows that the quasi-harmonic idealization, for the limiting case where the Grüneisen function approaches zero, actually approaches the harmonic approximation.

In a subsequent report, the author intends to address how real material behavior may be described in the framework of Segletes' equation of state, by departing from the quasi-harmonic idealization, and how, as lattice spacing increases, the quasi-harmonic idealization is approached for real lattices. Such a result is wholly compatible with the conclusions of Plendl [11], who asserts that anharmonicity is "mainly caused by the forces of repulsion..., but is close to zero when ions deviate from one another," (*i.e.*, when $\lambda > \lambda_0$).

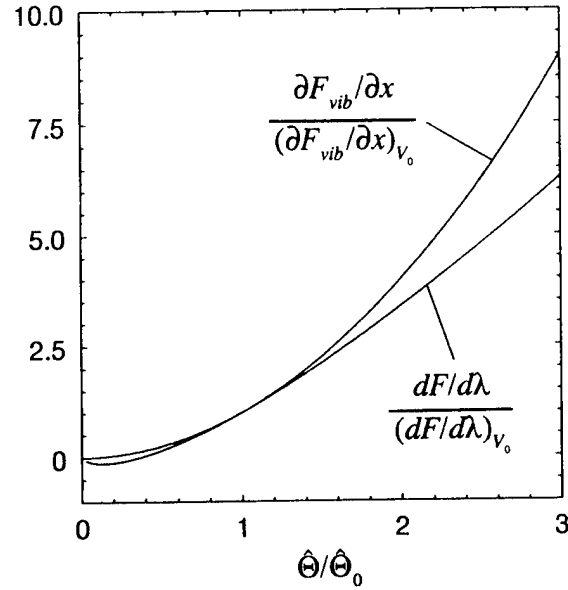


Figure 1. Relative values of the vibrational ($\partial F_{vib}/\partial x$) and volumetric ($dF/d\lambda$) stiffnesses, as a function of the relative characteristic temperature (or frequency), for a material obeying the quasi-harmonic idealization.

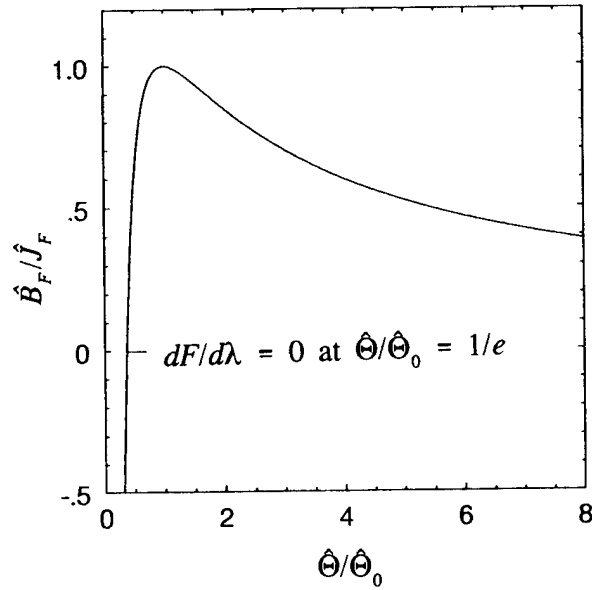


Figure 2. Ratio of volumetric to vibrational (force-based) moduli, as a function of the relative characteristic temperature (or frequency), for a material obeying the quasi-harmonic idealization.

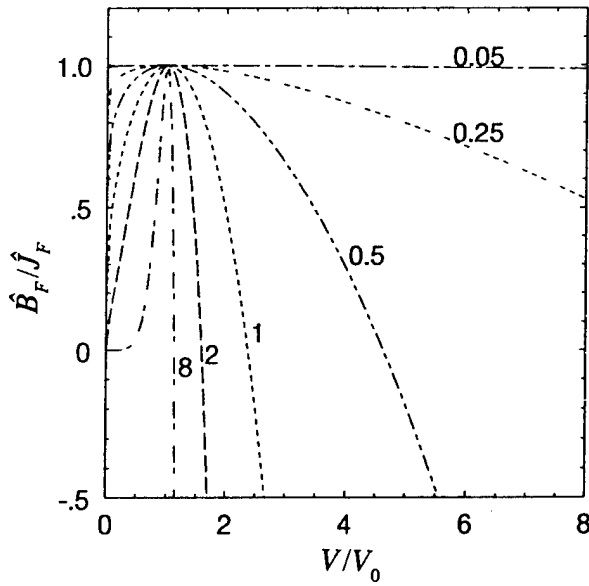


Figure 3. Ratio of volumetric to vibrational (force-based) moduli, as a function of relative volume, for a material obeying the quasi-harmonic idealization. Six curves are shown, corresponding to different values of the reference Grüneisen parameter, Γ_0 .

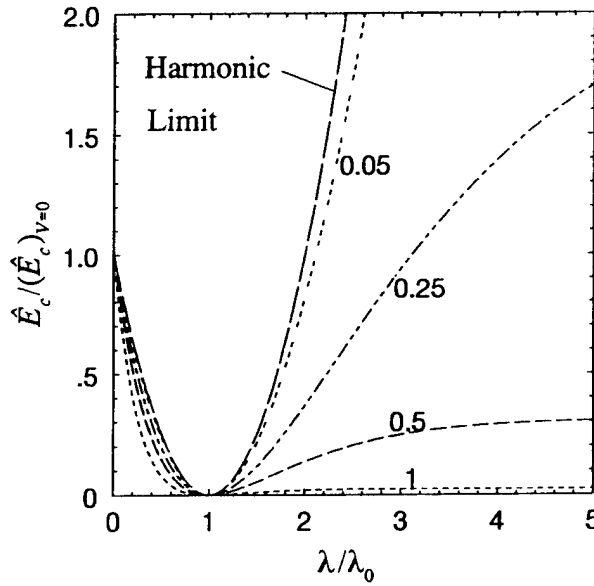


Figure 4. Relative cold compression energy versus relative lattice spacing, with reference Grüneisen value, Γ_0 , as a parameter, for quasi-harmonic material. As Γ_0 approaches zero, harmonicity is approached.

6. References

1. Born, M. and T. von Karman. "Über Schwingungen in Raumgittern." *Physikalische Zeitschrift*, **13** (8), pp. 297–309, 1912.
2. Brillouin, L. *Wave Propagation in Periodic Structures*. New York: Dover, 1953. Originally published by New York: McGraw Hill, 1946.
3. Rose, J. H., J. R. Smith, F. Guinea, and J. Ferrante. "Universal Features of the Equation of State of Metals." *Physical Review B*, **29** (6), pp. 2963–2969, 1984.
4. Blackman, M. "The Specific Heat of Solids." In *Encyclopedia of Physics; Volume VII Part 1: Crystal Physics I*. S. Flügge (ed.), Berlin: Springer-Verlag, pp. 325–382, 1955.
5. Barron, H. T. K. "On the Thermal Expansion of Solids at Low Temperatures." *Philosophical Magazine*, **46**, pp. 720–734, 1955.
6. Grodzka, P. G. "Grüneisen Parameter Study." Lockheed Missile Space Company Report LMSC/HREC A784868, Huntsville, AL, 1967.
7. Slater, J. C. *Introduction to Chemical Physics*. New York: McGraw Hill, 1939.
8. Dugdale, J. S. and D. K. C. MacDonald. "The Thermal Expansion of Solids." *Physical Review*, **89** (4), pp. 832–834, 1953.
9. Pastine, D. J. "Formulation of the Grüneisen Parameter for Monatomic Cubic Crystals." *Physical Review*, **138** (3A), pp. A767–A770, 1965.
10. Vashchenko, V. Y. and V. N. Zubarev. "Concerning the Grüneisen Constant." *Soviet Physics—Solid State*, **5** (3), pp. 653–655, 1963.
11. Plendl, J. N. "New Concepts in the Physics of Solids: A Monograph." Air Force Cambridge Research Laboratories Report AFCRL-66-541, Bedford, Massachusetts, August 1966.

12. Guinea, F., J. H. Rose, J. R. Smith, and J. Ferrante. "Scaling Relations in the Equation of State, Thermal Expansion, and Melting of Metals." *Applied Physics Letters*, **44** (1), pp. 53–55, 1984.
13. Segletes, S. B. "An Equation of State for Metals." ARL-TR-1270, U.S. Army Research Laboratory, Aberdeen Proving Ground, Maryland, November, 1996.
14. Segletes, S. B. "An Equation of State for Metals." under consideration by the *Journal of Applied Physics*, 1997.
15. Vinet, P., J. R. Smith, J. Ferrante, and J. H. Rose. "Temperature Effects on the Universal Equation of State for Solids." *Physical Review B*, **35** (4), pp. 1945–1953, 1987.
16. Vinet, P., J. H. Rose, J. Ferrante, and J. R. Smith. "Universal Features of the Equation of State of Solids." *Journal of Physics: Condensed Matter*, **1**, pp. 1941–1963, 1989.
17. Baonza, V. G., M. Cáceres, and J. Núñez. "Universal Compressibility Behavior of Dense Phases." *Physical Review B*, **51** (1), pp. 28–37, 1995.
18. Baonza, V. G., M. Taravillo, M. Cáceres, and J. Núñez. "Universal Features of the Equation of State of Solids from a Pseudospinodal Hypothesis." *Physical Review B*, **53** (9), pp. 5252–5258, 1996.
19. Segletes, S. B. "Further Examinations on the Thermodynamic Stability of the Mie-Grüneisen Equation of State." *Journal of Applied Physics*, **76** (8), pp. 4560–4566, 1994.
20. Segletes, S. B. "The Effect of Thermodynamic Constraints upon the Mie-Grüneisen Equation of State." in *Constitutive Laws*. A. M. Rajendran, R. C. Batra (eds.), Barcelona: CIMNE, pp. 46–51, 1995.
21. Segletes, S. B. and W. P. Walters. "On Theories of the Grüneisen Parameter." ARL-TR-1303, U.S. Army Research Laboratory, Aberdeen Proving Ground, Maryland, March, 1997.

22. Segletes, S. B. and W. P. Walters. "On Theories of the Grüneisen Parameter." *Journal of Physics and Chemistry of Solids*, to appear, 1997.
23. Kittel, C. *Introduction to Solid State Physics*. Third Edition, New York: Wiley, 1967.

INTENTIONALLY LEFT BLANK.

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
2	DEFENSE TECHNICAL INFORMATION CENTER ATTN DTIC DDA 8725 JOHN J KINGMAN RD STE 0944 FT BELVOIR VA 22060-6218
1	HQDA DAMO FDQ ATTN DENNIS SCHMIDT 400 ARMY PENTAGON WASHINGTON DC 20310-0460
1	US MILITARY ACADEMY MATH SCI CTR OF EXCELLENCE DEPT OF MATHEMATICAL SCI ATTN MDN A MAJ DON ENGEN THAYER HALL WEST POINT NY 10996-1786
1	DIRECTOR US ARMY RESEARCH LAB ATTN AMSRL CS AL TP 2800 POWDER MILL RD ADELPHI MD 20783-1145
1	DIRECTOR US ARMY RESEARCH LAB ATTN AMSRL CS AL TA 2800 POWDER MILL RD ADELPHI MD 20783-1145
3	DIRECTOR US ARMY RESEARCH LAB ATTN AMSRL CI LL 2800 POWDER MILL RD ADELPHI MD 20783-1145
<u>ABERDEEN PROVING GROUND</u>	
2	DIR USARL ATTN AMSRL CI LP (305)

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	US ARMY DUSA OPS RSCH ATTN DANIEL WILLARD 102 ARMY PENTAGON WASHINGTON DC 20310-0102
1	MIT LINCOLN LAB ARMY SCIENCE BOARD ATTN WADE M KORNEGAY 244 WOOD ST RM S2 139 LEXINGTON MA 02173
5	DEFENSE NUCLEAR AGENCY ATTN MAJ JAMES LYON CDR KENNETH W HUNTER TONY FREDERICKSON R JEFFREY LAWRENCE SPSP KIM KIBONG 6801 TELEGRAPH RD ALEXANDRIA VA 22310-3398
3	COMMANDER US ARMY ARDEC ATTN AMSTA AR FSA E W P DUNN J PEARSON E BAKER PICATINNY ARSENAL NJ 07806-5000
1	COMMANDER US ARMY ARDEC ATTN AMSTA AR CCH V M D NICOLICH PICATINNY ARSENAL NJ 07806-5000
1	COMMANDER US ARMY ARDEC ATTN E ANDRICOPOULOS PICATINNY ARSENAL NJ 07806-5000
1	COMMANDER USA STRATEGIC DEFNS CMD ATTN CSSD H LL T CROWLES HUNTSVILLE AL 35807-3801
2	COMMANDER US ARMY MICOM ATTN AMSMI RD ST WF D LOVELACE M SCHEXNAYDER REDSTONE ARSENAL AL 35898-5250

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	MIS DEFNS & SPACE TECHNOLOGY ATTN CSSD SD T KENNETH H JORDAN PO BOX 1500 HUNTSVILLE AL 34807-3801
4	COMMANDER US ARMY BELVOIR RD&E CTR ATTN STRBE NAE B WESTLICH STRBE JMC T HANSHAW STRBE NAN S G BISHOP J WILLIAMS FORT BELVOIR VA 22060-5166
3	COMMANDER US ARMY RESEARCH OFFICE ATTN J CHANDRA K IYER J BAILEY PO BOX 12211 RESEARCH TRIANGLE PARK NC 27709-2211
1	NAVAL RESEARCH LABORATORY ATTN ANDREW E WILLIAMS CODE 6684 4555 OVERLOOK AVE SW WASHINGTON DC 20375
1	DIRECTOR NAVAL CIVIL ENGRNG LAB ATTN J YOUNG CODE L56 PORT HUENEME CA 93043
1	NAVAL POSTGRADUATE SCHOOL PHYSICS DEPARTMENT ATTN JOSEPH STERNBERG MONTEREY CA 93943
1	NAVAL AIR WARFARE CTR ATTN STEPHEN A FINNEGAN BOX 1018 RIDGECREST CA 93556
3	COMMANDER NAVAL WEAPONS CENTER ATTN T T YEE CODE 3263 D THOMPSON CODE 3268 W J MCCARTER CODE 6214 CHINA LAKE CA 93555

NO. OF
COPIES ORGANIZATION

9 COMMANDER
NAVAL SURFACE WARFARE CTR
DAHLGREN DIVISION
ATTN C R GARRETT CODE G22
W HOLT CODE G22
CHARLES R ELLINGTON
W WALLACE MORTON JR
JOHN M NELSON
WILLIAM J STROTHER
D L DICKINSON CODE G24
L F WILLIAMS CODE G33
M J SILL CODE H11
17320 DAHLGREN RD
DAHLGREN VA 22448-5000

13 COMMANDER
NAVAL SURFACE WARFARE CTR
ATTN D TASKER CODE 9220
W WILSON
P C HUANG CODE G402
B A BAUDLER CODE R12
R H MOFFETT CODE R12
R GARRETT CODE R12
T L JUNGLING CODE R32
R DAMINITY CODE U43
J P MATRA
P WALTER
L MENSİ
K KIDDY
F J ZERILLI
10901 NEW HAMPSHIRE AVE
SILVER SPRING MD 20903-5000

5 AIR FORCE ARMAMENT LAB
ATTN AFATL DLJW
W COOK
M NIXON
AFATL DLJR J FOSTER
AFATL MNW
LT D LOREY
R D GUBA
EGLIN AFB FL 32542

NO. OF
COPIES ORGANIZATION

5 WRIGHT LABS
ATTN MNMW JOEL W HOUSE
ARMAMENT DIRECTORATE STE 326 B1
RONALD D HUNT
BRYAN MILLIGAN
BRUCE C PATTERSON
WADE H VAUGHT
101 W EGLIN BLVD
EGLIN AFB FL 32542-6810

2 USAF PHILLIPS LABORATORY
ATTN PL WSCD FIROOZ ALLAHDAI
PV VTA DAVID SPENCER
3550 ABERDEEN AVE SE
KIRTLAND AFB NM 87117-5776

1 USAF PHILLIPS LABORATORY
VTSI
ATTN ROBERT ROYBAL
KIRTLAND AFB NM 87117-7345

1 AFIT ENC
ATTN DAVID A FULK
WRIGHT PATTERSON AFB OH 45433

1 US DEPT OF ENERGY
IDAHO OPERATIONS OFFICE
ATTN RONALD H JOHNSON
850 ENERGY DR
IDAHO FALLS ID 83401-1563

5 DIRECTOR
LANL
ATTN J MCAFEE MS P950
D PAISLEY MS P950
L PICKLESIMER MS P950
R WARNES MS P950
S SHEFFIELD MS P952
PO BOX 1663
LOS ALAMOS NM 87545

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
43	DIRECTOR LANL ATTN M LUCERO MS A105 D MANDELL K MARK JOSEPH V REPA MS A133 MICHAEL O SCHNICK MS F607 EDWARD J CHAPYAK MS F664 J P RITCHIE MS B214 T14 R DINGUS MS B218 N KRIKORIAN MS B228 R KIRKPATRICK MS B229 R THURSTON MS B229 C T KLINGNER MS B294 R MILLER MS B294 S J MOSSO B SHAFER MS C931 G GISLER MS D436 C RAGAN MS D449 B LAUBSCHER MS D460 R WELLS MS F607 R KOPP MS F645 R STELLINGWERF MS F645 C WINGATE MS F645 T ADAMS MS F663 R GODWIN MS F663 K JACOBY MS F663 W SPARKS MS F663 J SHANER MS F670 G CANAVAN MS F675 R GREINER MS G740 J HILLS MS G770 B HOGAN MS G770 J BOLSTAD MS G787 J WALSH MS G787 R DAVIDSON MS K557 R HENNINGER MS K557 N6 T ROLLET MS K574 P HOWE MS P915 W DEAL MS P915 J KENNEDY MS P915 A ROACH MS P915 L SCHWALBE W HEMSING MS P940 E POGUE MS P940 PO BOX 1663 LOS ALAMOS NM 87545

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
41	DIRECTOR LLNL ATTN R E TIPTON L35 D BAUM L35 T MCABEE MS 35 M J MURPHY R PIERCE L122 R ROSINKY L122 O J ALFORD L122 D STEWART L122 T VIDLAK L122 B R BOWMAN L122 W DIXON L122 A C MITCHELL J A MORIARTY R A HEINLE N C HOLMES R PERRET L163 W SHOTTS L163 H KRUGER L178 G POMYKAL L178 M SHANNON G SIMONSON L180 A SPERO L180 W TAO L282 P URTIEW L282 A HOLT L290 J E REAUGH L290 W J NELLIS L299 D WOOD L352 D GAVEL L495 J HUNTER L495 E JOHANSSON L495 R M KUKLO L874 G W REPP DOUGLAS R FAUX L125 NORMAN W KLINO L125H ROBERT BARKER L159 MILTON FINGER L163 MICHAEL GERASSIMENKO L178 FRANK A HANDLER L182 STEPHEN G COCHRAN L389 BMDO ROBERT M HALL PO BOX 808 LIVERMORE CA 94550

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
44	DIRECTOR SANDIA NATL LABS ATTN E S HERTEL JR MS-0819 A ROBINSON MS-0819 L N KMETYK E H BARSIS MS-031 ERIC W REECE MS-0307 DANIEL P KELLY MS-0307 L WEIRICK MS-0327 R TACHAU MS-0425 D LONGCOPE MS-0439 R REEDER D HAYES MS-0457 J ASAY MS-0458 W TEDESCHI MS-0482 J SCHULZE MS-0483 J SOUTHWARD PAUL A LONGMIRE MS-0560 T TRUCANO MS-0819 J MICHAEL MCGLAUN MS-0819 R BRANNON MS-0820 J ANG MS-0821 M BOSLOUGH MS-0821 L CHHABILDAS MS-0821 D CRAWFORD MS-0821 J DICK M FURNISH MS-0821 C HALL MS-0821 W REINHART MS-0821 P STANTON MS-0821 P TAYLOR ORG 1432 D KERNAN ORG 1433 C KONRAD K LANG M KIPP DIV 1533 P YARRINGTON DIV 1533 J MCGLAWA DIV 1541 M FORRESTAL DIV 1551 R GRAHAM DIV 1551 R LAFARGE DIV 1551 C HILLS DIV 1822 W J ANDRZEJEWSKI DIV 2512 D MARCHI DIV 2512 W VANDERMOLLEN ORG 2653 B LEVIN ORG 7816 R O NELLUMS DIV 9122 PO BOX 5800 ALBUQUERQUE NM 87185

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
3	ENERGETIC MATERIALS RSCH CTR/DOE NEW MEXICO INST OF MINING & TECH ATTN DAVID J CHAVEZ LARRY LIBERSKY FRED SANDSTROM CAMPUS STATION SOCORRO NM 87801
1	NASA LEWIS RESEARCH CENTER ATTN J FERRANTE CLEVELAND OH 44135
3	NASA JOHNSON SPACE CENTER ATTN ERIC CHRISTIANSEN JEANNE LEE CREWS FREDRICH HORZ MAIL CODE SN3 2101 NASA RD 1 HOUSTON TX 77058
1	APPLIED RESEARCH LAB ATTN JEFFREY A COOK 10000 BURNETT ROAD AUSTIN TX 78758
1	GM RESEARCH LABS ATTN J R SMITH WARREN MI 48090
5	JET PROPULSION LABORATORY IMPACT PHYSICS GROUP ATTN ZDENEK SEKANINA PAUL WEISSMAN BOB WEST JAMES ZWISSLER MARC ADAMS 4800 OAK GROVE DR PASADENA CA 91109
1	MAXWELL LABS S CUBED DIVISION ATTN GERALD A GURTMAN PO BOX 1620 LA JOLLA CA 92037

NO. OF
COPIES ORGANIZATION

1 BROWN UNIVERSITY
DIV OF ENGINEERING
ATTN R CLIFTON
PROVIDENCE RI 02912

2 CALTECH
ATTN ANDREW P INGERSOLL MS 170 25
THOMAS J AHRENS MS 252 21
1201 E CALIFORNIA BLVD
PASADENA CA 91125

1 CALTECH
ATTN GLENN ORTON MS 169 237
4800 OAK GROVE DR
PASADENA CA 91007

1 DREXEL UNIVERSITY
ATTN PHYSICS DEPT
32ND & CHESTNUT ST
PHILADELPHIA PA 19104

1 GEORGIA INSTITUTE OF TECHNOLOGY
COMPUTATIONAL MODELING CENTER
ATTN S ATLURI
ATLANTA GA 30332-0356

1 GEORGIA INSTITUTE OF TECHNOLOGY
SCHOOL OF MATL SCIENCE & ENGNG
ATTN K LOGAN
ATLANTA GA 30332-0245

1 IOWA STATE UNIVERSITY
DEPT PHYSICS AND ASTRONOMY
ATTN JIM ROSE
34 PHYSICS
AMES IA 50011

5 JOHNS HOPKINS UNIV
APPLIED PHYSICS LAB
ATTN TERRY R BETZER
ALVIN R EATON
RICHARD H KEITH
DALE K PACE
ROGER L WEST
JOHNS HOPKINS ROAD
LAUREL MD 20723

NO. OF
COPIES ORGANIZATION

1 LOUISIANA STATE UNIVERSITY
ATTN ROBERT W COURTER
948 WYLIE DR
BATON ROUGE LA 70808

1 MIT DEPT OF EARTH ATMOS AND
PLANETARY SCIENCES
ATTN HEIDI B HAMMELL 54 316
CAMBRIDGE MA 02139

1 NC STATE UNIVERSITY
ATTN YASUYUKI HORIE
RALEIGH NC 27695-7908

1 PENNSYLVANIA STATE UNIVERSITY
ATTN PHYSICS DEPT
UNIVERSITY PARK PA 16802

5 SOUTHWEST RESEARCH INSTITUTE
ATTN C ANDERSON
S A MULLIN
B COUR PALAIS
J RIEGEL
J WALKER
PO DRAWER 28510
SAN ANTONIO TX 78284

1 TEXAS A&M UNIVERSITY
PHYSICS DEPARTMENT
ATTN DAN BRUTON
COLLEGE STATION TX 77843-4242

1 UC BERKELEY
MECHANICAL ENGINEERING DEPT
GRADUATE OFFICE
ATTN KEZHUN LI
BERKELEY CA 94720

1 UC DAVIS
INST OF THEORETICAL DYNAMICS
ATTN E G PUCKETT
DAVIS CA 95616

1 UC LOS ANGELES
DEPT OF MAT SCIENCE & ENGNG
ATTN J J GILMAN
LOS ANGELES CA 90024

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>	<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
2	UC SAN DIEGO DEPT APPL NECH & ENGR SVCS R011 ATTN S NEMAT-NASSER M MEYERS LA JOLLA CA 92093-0411	1	UNIVERSITY OF TEXAS DEPT OF MECHANICAL ENGINEERING ATTN ERIC P FAHRENTHOLD AUSTIN TX 78712
2	UNIV OF ALA HUNTSVILLE AEROPHYSICS RSCH CTR ATTN GARY HOUGH DAVID J LIQUORNIK PO BOX 999 HUNTSVILLE AL 35899	1	VIRGINIA POLYTECHNIC INSTITUTE COLLEGE OF ENGINEERING ATTN R BATRA BLACKSBURG VA 24061-0219
1	UNIV OF ALA HUNTSVILLE CIVIL ENGRNG DEPT ATTN WILLIAM P SCHONBERG HUNTSVILLE AL 35899	2	AEROJET ATTN J CARLEONE S KEY PO BOX 13222 SACRAMENTO CA 95813-6000
1	UNIVERSITY OF CHICAGO DEPT OF THE GEOPHYSICAL SCIENCES ATTN G H MILLER 5734 S ELLIS AVE CHICAGO IL 60637	2	AEROJET ORDNANCE ATTN P WOLF G PADGETT 1100 BULLOCH BLVD SOCORRO NM 87801
3	UNIVERSITY OF DAYTON RSCH INST KLA14 ATTN N BRAR D GROVE A PIEKUTOWSKI 300 COLLEGE PARK DAYTON OH 45469-0182	3	ALLIANT TECHSYSTEMS INC ATTN T HOLMQUIST MN11 2720 R STRYK G R JOHNSON MN11 2925 600 SECOND ST NE HOPKINS MN 55343
4	UNIVERSITY OF DELAWARE DEPT OF MECHANICAL ENGINEERING ATTN PROF J GILLESPIE DEAN R B PIPES PROF J VINSON PROF D WILKINS NEWARK DE 19716	1	ALME AND ASSOCIATES ATTN MARVIN L ALME 6219 BRIGHT PLUME COLUMBIA MD 21044-3790
1	UNIVERSITY OF MARYLAND ATTN PHYSICS DEPT (BLDG 082) COLLEGE PARK MD 20742	1	APPLIED RESEARCH ASSOC INC ATTN JEROME D YATTEAU 5941 S MIDDLEFIELD RD SUITE 100 LITTLETON CO 80123
1	UNIVERSITY OF PUERTO RICO DEPT CHEMICAL ENGINEERING ATTN L A ESTEVEZ MAYAGUEZ PR 00681-5000	2	APPLIED RESEARCH ASSOC INC ATTN DENNIS GRADY FRANK MAESTAS 4300 SAN MATEO BLVD SE ALBUQUERQUE NM 87110
		1	BATTELLE ATTN ROBER M DUGAS 7501 S MEMORIAL PKWY SUITE 101 HUNTSVILLE AL 35802-2258

NO. OF
COPIES ORGANIZATION

3 BOEING AEROSPACE CO
SHOCK PHYSICS & APPLIED MATH
ENGINEERING TECHNOLOGY
ATTN R HELZER
T MURRAY
J SHRADER
PO BOX 3999
SEATTLE WA 98124

1 BOEING HOUSTON SPACE STN
ATTN RUSSELL F GRAVES
BOX 58747
HOUSTON TX 77258

1 BRIGS CO
ATTN JOSEPH E BACKOFEN
2668 PETERSBOROUGH ST
HERNDON VA 20171-2443

1 CALIFORNIA RSCH & TECHNOLOGY
ATTN M MAJERUS
PO BOX 2229
PRINCETON NJ 08543

1 CENTURY DYNAMICS INC
ATTN N BIRNBAUM
2333 SAN RAMON VALLEY BLVD
SAN RAMON CA 94583-1613

1 COMPUTATIONAL MECHANICS
CONSULTANTS
ATTN J A ZUKAS
PO BOX 11314
BALTIMORE MD 21239-0314

1 CYPRESS INTERNATIONAL
ATTN A CAPONECCHI
1201 E ABINGDON DR
ALEXANDRIA VA 22314

1 DEFENSE TECHNOLOGY INTL. INC
ATTN D E AYER
THE STARK HOUSE
22 CONCORD ST
NASHUA NH 03060

1 DESKIN RESEARCH GROUP INC
ATTN EDWARD COLLINS
2270 AGNEW RD
SANTA CLARA CA 95054

NO. OF
COPIES ORGANIZATION

1 DOW CHEMICAL INC
ORDNANCE SYSTEMS
ATTN C HANEY
A HART
B RAFANIELLO
800 BUILDING
MIDLAND MI 48667

1 G E DUVALL
5814 NE 82ND COURT
VANCOUVER WA 98662-5944

3 DYNA EAST CORP
ATTN P C CHOU
R CICCARELLI
W FLIS
3620 HORIZON DRIVE
KING OF PRUSSIA PA 19406

3 DYNASEN
ATTN JACQUES CHAREST
MICHAEL CHAREST
MARTIN LILLY
20 ARNOLD PL
GOLETA CA 93117

1 R J EICHELBERGER
409 W CATHERINE ST
BEL AIR MD 21014-3613

1 ELORET INSTITUTE
ATTN DAVID W BOGDANOFF MS 230 2
NASA AMES RESEARCH CENTER
MOFFETT FIELD CA 94035

3 ENIG ASSOCIATES INC
ATTN J ENIG
D J PASTINE
M COWPERTHWAIT
SUITE 500
11120 NEW HAMPSHIRE AVE
SILVER SPRING MD 20904-2633

1 EXPLOSIVE TECHNOLOGY
ATTN M L KNAEBEL
PO BOX KK
FAIRFIELD CA 94533

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	GB TECH LOCKHEED ATTN JAY LAUGHMAN 2200 SPACE PARK SUITE 400 HOUSTON TX 77258
2	GB TECH LOCKHEED ATTN LUCILLE BORREGO C23C JOE FALCON JR C23C 2400 NASA ROAD 1 HOUSTON TX 77058
6	GDLS 38500 MOUND RD ATTN W BURKE MZ436-21-24 G CAMPBELL MZ436-30-44 D DEBUSSCHER MZ436-20-29 J ERIDON MZ436-21-24 W HERMAN MZ 435-01-24 S PENTESCU MZ436-21-24 STERLING HTS MI 48310-3200
2	GENERAL RESEARCH CORP ATTN A CHARTERS T MENNA PO BOX 6770 SANTA BARBARA CA 93160-6770
2	GRC INTERNATIONAL ATTN TIMOTHY M CUNNINGHAM WILLIAM M ISBELL 5383 HOLLISTER AVE SANTA BARBARA CA 93111
6	INST OF ADVANCED TECHNOLOGY UNIVERSITY OF TX AUSTIN ATTN STEPHEN J BLESS JAMES CAZAMIAS HARRY D FAIR THOMAS M KIEHNE DAVID LITTLEFIELD MIKE NORMANDIA 4030-2 W BRAKER LN AUSTIN TX 78759
1	INTERNATIONAL RESEARCH ASSOC ATTN D ORPHAL 4450 BLACK AVE PLEASANTON CA 94566

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	INTERPLAY ATTN F E WALKER 18 SHADOW OAK RD DANVILLE CA 94526
1	KAMAN SCIENCES CORP ATTN DENNIS L JONES 2560 HUNTINGTON AVE SUITE 200 ALEXANDRIA VA 22303
8	KAMAN SCIENCES CORP ATTN J ELDER RICHARD P HENDERSON DAVID A PYLES FRANK R SAVAGE JAMES A SUMMERS JAMES S WILBECK TIMOTHY W MOORE THY YEM 600 BLVD S SUITE 208 HUNTSVILLE AL 35802
3	KAMAN SCIENCES CORP ATTN SHELDON JONES GARY L PADEREWSKI ROBERT G PONZINI 1500 GRDN OF THE GODS RD COLORADO SPRINGS CO 80907
4	KAMAN SCIENCES CORP ATTN NASIT ARI STEVE R DIEHL WILLIAM DOANE VERNON M SMITH PO BOX 7463 COLORADO SPRINGS CO 80933-7463
1	D R KENNEDY & ASSOC INC ATTN D KENNEDY PO BOX 4003 MOUNTAIN VIEW CA 94040
1	KERLEY PUBLISHING SERVICES ATTN G I KERLEY PO BOX 13835 ALBUQUERQUE NM 87192-3835

NO. OF
COPIES ORGANIZATION

2 KTECH CORPORATION
ATTN FRANK W DAVIES
LARRY M LEE
901 PENNSYLVANIA NE
ALBUQUERQUE NM 87110

1 LIVERMORE SOFTWARE TECH CORP
ATTN J O HALLQUIST
2876 WAVERLY WAY
LIVERMORE CA 94550

1 LOCKHEED MARTIN MISSILE & SPACE
ATTN WILLIAM R EBERLE
PO BOX 070017
HUNTSVILLE AL 35807

3 LOCKHEED MARTIN MISSILE & SPACE
ATTN M A LEVIN ORG 81 06 BLDG 598
M R MCHENRY
T A NGO ORG 81 10 BLDG 157
111 LOCKHEED WAY
SUNNYVALE CA 94088

4 LOCKHEED MISSILE & SPACE CO
ATTN JOHN R ANDERSON
WILLIAM C KNUDSON
S KUSUMI 0 81 11 BLDG 157
J PHILLIPS 0 54 50
PO BOX 3504
SUNNYVALE CA 94088

1 LOCKHEED MISSILE & SPACE CO
ATTN R HOFFMAN
SANTA CRUZ FACILITY
EMPIRE GRADE RD
SANTA CRUZ CA 95060

1 LOCKHEED NASA JSC
SPACE SCIENCE BRANCH
ATTN JAMES HYDE
BOX 58561 MC B22
HOUSTON TX 77258

1 LOCKHEED MARTIN AEROSPACE
ATTN D R BRAGG
PO BOX 5837 MP 109
ORLANDO FL 32855

NO. OF
COPIES ORGANIZATION

1 MCDONNELL DOUGLAS
ASTRONAUTICS CO
ATTN B L COOPER
5301 BOLSA AVE
HUNTINGTON BEACH CA 92647

1 ORLANDO TECHNOLOGY INC
ATTN DANIEL A MATUSKA
PO BOX 855
SHALIMAR FL 32579

1 PHYSICAL SCIENCES INC
ATTN PETER NEBOLSINE
20 NEW ENGLAND BUS CTR
ANDOVER MA 01810

3 PHYSICS INTERNATIONAL
ATTN R FUNSTON
G FRAZIER
L GARNETT
PO BOX 5010
SAN LEANDRO CA 94577

1 PRC INC
ATTN J ADAMS
5166 POTOMAC DR #103
KING GEORGE VA 22485-5824

1 RAYTHEON ELECTRONIC SYSTEMS
ATTN R KARPP
50 APPLE HILL DRIVE
TEWKSBURY MA 01876

1 ROCKWELL INTERNATIONAL
ROCKETDYNE DIVISION
ATTN H LEIFER
16557 PARK LN CIRCLE
LOS ANGELES CA 90049

1 ROCKWELL MISSILE SYS DIV
ATTN T NEUHART
1800 SATELLITE BLVD
DULUTH GA 30136

2 SAIC
ATTN JAMES FURLONG
GREGORY J STRAUCH
1710 GOODRIDGE DR
MCLEAN VA 22102

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	SAIC ATTN MICHAEL W MCKAY 10260 CAMPUS POINT DR SAN DIEGO CA 92121
1	SHOCK TRANSIENTS INC ATTN DAVID DAVISON BOX 5357 HOPKINS MN 55343
2	SIMULATION & ENG CO INC ATTN ELSA I MULLINS STEVEN E MULLINS 8840 HWY 20 SUITE 200 N MADISON AL 35758
2	SOUTHERN RESEARCH INSTITUTE ATTN LINDSEY A DECKARD DONALD P SEGERS PO BOX 55305 BIRMINGHAM AL 35255-5305
5	SRI INTERNATIONAL ATTN JAMES D COLTON D CURRAN R KLOOP R L SEAMAN D A SHOCKEY 333 RAVENSWOOD AVE MENLO PARK CA 94025
2	TELEDYNE BROWN ENGR ATTN JIM W BOOTH MARTIN B RICHARDSON PO BOX 070007 MS 50 HUNTSVILLE AL 35807-7007
1	ZERNOW TECHNICAL SVCS INC ATTN LOUIS ZERNOW 425 W BONITA AVE SUITE 208 SAN DIMAS CA 91773

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
	ABERDEEN PROVING GROUND
30	DIR, USARL ATTN: AMSRL-WM, I MAY AMSRL-WM-MF, S CHOU D DANDEKAR A RAJENDRAN AMSRL-WM-PB, A ZIELINSKI AMSRL-WM-PD, G GAZONAS AMSRL-WM-T, W F MORRISON AMSRL-WM-TA, M BURKINS W GILLICH W BRUCHEY J DEHN G FILBEY W A GOOCH H W MEYER E J RAPACKI J RUNYEON AMSRL-WM-TB, R FREY P BAKER J STARKENBERG AMSRL-WM-TC, W S DE ROSSET T W BJERKE R COATES F GRACE K KIMSEY M LAMPSON D SCHEFFLER S SCHRAML B SORENSEN R SUMMERS W WALTERS

NO. OF
COPIES ORGANIZATION

15 DIR, USARL
 AMSRL-WM-TD,
 A M DIETRICH
 K FRANK
 J HARRISON
 M RAFTENBERG
 G RANDERS-PEHRSON
 M SCHEIDLER
 S SCHOENFELD
 S SEGLETES (5 CP)
 J WALTER
 T WRIGHT
 AMSRL-WM-WD, A PRAKASH

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
3	AERONAUTICAL & MARITIME RESEARCH LABORATORY ATTN N BURMAN S CIMPOERU D PAUL PO BOX 4331 MELBOURNE VIC 3001 AUSTRALIA
1	EMBASSY OF AUSTRALIA ATTN R WOODWARD COUNSELLOR DEFENCE SCIENCE 1601 MASSACHUSETTS AVE NW WASHINGTON DC 20036-2273
1	ABTEILUNG FUER PHYSIKALISCHE CHEMIE MONTANUNIVERSITAET ATTN E KOENIGSBERGER A 8700 LEOBEN AUSTRIA
1	PRB S A ATTN M VANSNICK AVENUE DE TERVUEREN 168 BTE 7 BRUSSELS B 1150 BELGIUM
1	ROYAL MILITARY ACADEMY ATTN E CELENS RENAISSANCE AVE 30 B1040 BRUSSELS BELGIUM
1	BULGARIAN ACADEMY OF SCIENCES SPACE RESEARCH INSTITUTE ATTN VALENTIN GOSPODINOV 1000 SOFIA PO BOX 799 BULGARIA
1	CANADIAN ARSENALS LTD ATTN P PELLETIER 5 MONTEE DES ARSENAUX VILLIE DE GRADEUR PQ J5Z2 CANADA
1	DEFENCE RSCH ESTAB SUFFIELD ATTN D MACKAY RALSTON ALBERTA T0J 2N0 RALSTON CANADA

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	DEFENCE RSCH ESTAB SUFFIELD ATTN CHRIS WEICKERT BOX 4000 MEDICINE HAT ALBERTA T1A 8K6 CANADA
1	DEFENCE RSCH ESTAB VALCARTIER ARMAMENTS DIVISION ATTN R DELAGRAVE 2459 PIE X1 BLVD N PO BOX 8800 CORCELETTE QUEBEC G0A 1R0 CANADA
1	UNIVERSITY OF GUELPH PHYSICS DEPT ATTN C G GRAY GUELPH ONTARIO N1G 2W1 CANADA
1	CEA ATTN ROGER CHERET CEDEX 15 313 33 RUE DE LA FEDERATION PARIS 75752 FRANCE
1	CEA CISI BRANCH ATTN PATRICK DAVID CENTRE DE SACLAY BP 28 GIF SUR YVETTE 91192 FRANCE
1	CEA/CESTA ATTN ALAIN GEILLE BOX 2 LE BARP 33114 FRANCE
6	CENTRE D'ETUDES DE GRAMAT ATTN SOLVE GERARD CHRISTIAN LOUPIAS PASCALE OUTREBON J CAGNOUX C GALLIC J TRANCHET GRAMAT 46500 FRANCE

NO. OF
COPIES ORGANIZATION

2 CENTRE D'ETUDES DE LIMEIL-VALENTON
ATTN CHRISTIAN AUSSOURD
JEAN-CLAUDE BOZIER
SAINT GEORGES CEDEX
VILLENEUVE 94195
FRANCE

3 CENTRE D'ETUDES DE VAUJOURS
ATTN PLOTARD JEAN-PAUL
ERIC BOTTET
TAT SIHN VONG
BOITE POSTALE NO 7
COUNTRY 77181
FRANCE

6 CENTRE DE RECHERCHES
ET D'ETUDES D'ARCUEIL
ATTN D BOUVART
C COTTENNOT
S JONNEAUX
H ORSINI
S SERROR
F TARDIVAL
16 BIS AVENUE PRIEUR DE
LA COTE D'OR
F94114 ARCUEIL CÉDEX
FRANCE

1 DAT ETBS CETAM
ATTN CLAUDE ALTMAYER
ROUTE DE GUERRY BOURGES
18015
FRANCE

1 ETBS DSTI
ATTN P BARNIER
ROUTE DE GUERAY
BOITE POSTALE 712
18015 BOURGES CEDEX
FRANCE

1 FRENCH GERMAN RESEARCH INST
ATTN CHANTERET P-Y
CEDEX 12 RUE DE L'INDUSTRIE
BP 301
F68301 SAINT-LOUIS
FRANCE

NO. OF
COPIES ORGANIZATION

5 FRENCH GERMAN RESEARCH INST
ATTN HANS-JURGEN ERNST
FRANCIS JAMET
PASCALE LEHMANN
K HOOG
H LERR
CEDEX 5 5 RUE DU GENERAL
CASSAGNOU
SAINT LOUIS 68301
FRANCE

1 LABORATOIRE DE TECHNOLOGIE DES
SURFACES
ECOLE CENTRALE DE LYON
ATTN VINET P
BP 163
69131 ECULLY CEDEX
FRANCE

1 BATTELLE INGENIEUTECHNIK GMBH
ATTN W FUCHE
DUESSELDORFFER STR 9
ESCHBORN D 65760
GERMANY

1 CONDAT
ATTN J KIERMEIR
MAXIMILIANSTR 28
8069 SCHEYERN FERNHAG
GERMANY

1 DEUTSCHE AEROSPACE AG
ATTN MANFRED HELD
POSTFACH 13 40
D 86523 SCHROBENHAUSEN
GERMANY

1 DIEHL GBMH AND CO
ATTN M SCHILDKNECHT
FISCHBACHSTRASSE 16
D 90552 RÖTBENBACH AD PEGNITZ
GERMANY

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
5	ERNST MACH INSTITUT ATTN VOLKER HOHLER E SCHMOLINSKE E SCHNEIDER A STILP K THOMA ECKERSTRASSE 4 D-7800 FREIBURG I BR 791 4 GERMANY
1	EUROPEAN SPACE AGENCY ATTN WALTER FLURY ESOC 5 ROBT BOSCHT STRASSE DARMSTADT 6100 GERMANY
3	FRAUNHOFER INSTITUT FUER KURZZEITDYNAMIK ERNST MACH INSTITUT ATTN H ROTHENHAEUSLER H SENF E STRASSBURGER HAUPTSTRASSE 18 D79576 WEIL AM RHEIN GERMANY
3	FRENCH GERMAN RESEARCH INST ATTN HARTMUTH F LEHR ROLF HUNKLER ERICH WOLLMANN POSTFACH 1260 WEIL AM RHEIN D-79574 GERMANY
2	IABG ATTN M BORRMANN H G DORSCH EINSTEINSTRASSE 20 D 8012 OTTOBRUN B MUENCHEN GERMANY
1	INGENIEURBÜRO DEISENROTH AUF DE HARDT 33 35 D5204 LOHMAR 1 GERMANY

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
3	TU CHEMNITZ-ZWICKAU ATTN I FABER L KRUEGER LOTHAR MEYER FAKULTAET FUER MASCHINENBAU U. VERFAHRENSTECHNIK SCHEFFELSTRASSE 110 09120 CHEMNITZ GERMANY
1	TECHNISCHE UNIVERSITAT MUENCHEN ATTN EDUARD B IGENBERGS RICHARD WAGNER STR 18 111 MUENCHEN 2 D8000 GERMANY
1	BHABHA ATOMIC RESEARCH CENTRE HIGH PRESSURE PHYSICS DIVISION ATTN N SURESH TROMBAY BOMBAY 400 085 INDIA
5	RAFAEL BALLISTICS CENTER ATTN EREZ DEKEL YEHUDA PARTOM G ROSENBERG Z ROSENBERG Y YESHURUN PO BOX 2250 HAIFA 31021 ISRAEL
1	TECHNION INST OF TECH FACULTY OF MECH ENGNG ATTN SOL BODNER TECHNION CITY HAIFA 32000 ISRAEL
1	CRC RESEARCH INST INC ATTN MASAHIDE KATAYAMA STRUCTURAL ENGINEERING DEPT 1 3 316 NAKASE MIHAMA KU CHIBA SHI 261 01 JAPAN

NO. OF
COPIES ORGANIZATION

- 1 ESTEC CS
ATTN DOUGLAS CASWELL
BOX 200 NOORDWIJK
2200 AG
NETHERLANDS
- 2 EUROPEAN SPACE AGENCY ESTEC
ATTN LUCY BERTHOUD
MICHEL LAMBERT
POSTBUS BOX 299 NOORDWIJK
NL2200 AG
NETHERLANDS
- 4 PRINS MAURITS LABORATORY
ATTN H J REITSMA
EDWARD VAN RIET
H PASMAN
R YSSELSTEIN
TNO BOX 45
RIJSWIJK 2280AA
NETHERLANDS
- 1 ROYAL NETHERLANDS ARMY
ATTN J HOENEVELD
V D BURCHLAAN 31
PO BOX 90822
2509 LS THE HAGUE
NETHERLANDS
- 4 HIGH ENERGY DENSITY RESEARCH CTR
ATTN VLADIMIR E FORTOV
GENADII I KANEL
V A SKVORTSOV
O YU VOJOBIEV
IZHORSKAJA STR 13/19
MOSCOW 127412
RUSSIAN REPUBLIC
- 1 INSTITUTE OF CHEMICAL PHYSICS
ATTN A YU DOLGOBORODOV
KOSYGIN ST 4 V 334
MOSCOW
RUSSIAN REPUBLIC

NO. OF
COPIES ORGANIZATION

- 3 INSTITUTE OF CHEMICAL PHYSICS
RUSSIAN ACADEMY OF SCIENCES
ATTN A M MOLODETS
S V RAZORENOV
A V UTKIN
142432 CHERNOGOLOVKA
MOSCOW REGION
RUSSIAN REPUBLIC
- 3 INSTITUTE OF MECH ENGINEERING PROBLEMS
ATTN V BULATOV
D INDEITSEV
Y MESCHERYAKOV
BOLSHOY, 61, V.O.
ST PETERSBURG 199178
RUSSIAN REPUBLIC
- 2 IOFFE PHYSICO TECHNICAL INSTITUTE
DENSE PLASMA DYNAMICS
LABORATORY
ATTN EDWARD M DROBYSHEVSKI
A KOZHUSHKO
ST PETERSBURG 194021
RUSSIAN REPUBLIC
- 1 IPE RAS
ATTN A A BOGOMAZ
DVORTSOVAIA NAB 18
ST PETERSBURG
RUSSIAN REPUBLIC
- 2 LAVRENTYEV INST. HYDRODYNAMICS
ATTN LEV A MERZHEVSKY
VICTOR V SILVESTROV
NOVOSIBIRSK 630090
RUSSIAN REPUBLIC
- 1 MOSCOW INST OF PHYSICS & TECH
ATTN S V UTUZHNIKOV
DEPT OF COMPUTATIONAL
MATHEMATICS
DOLGOPRUDNY 1471700
RUSSIAN REPUBLIC
- 1 RESEARCH INSTITUTE OF MECHANICS
NIZHNIY NOVGOROD STATE UNIVERSITY
ATTN A SADYRIN
P.R. GAYARINA 23 KORP 6
NIZHNIY NOVGOROD 603600
RUSSIAN REPUBLIC

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	SAMARA STATE AEROSPACE UNIV ATTN L G LUKASHEV SAMARA RUSSIAN REPUBLIC
1	TOMSK BRANCH OF THE INSTITUTE FOR STRUCTURAL MACROKINETICS ATTN V GORELSKI 8 LENIN SQ GSP 18 TOMSK 634050 RUSSIAN REPUBLIC
1	UNIVERSIDAD DE CANTABRIA FACULTAD DE CIENCIAS DEPARTAMENTO DE FISICA APLICADA ATTN J AMOROS AVDA DE LOS CASTROS S/N SANTANDER SPAIN
4	DEPARTAMENTO DE QUIMICA FISICA FACULTAD DE CIENCIAS QUIMICAS UNIVERSIDAD COMPLUTENSE DE MADRID ATTN V G BAONZA M TARAVILLO M CACERAS J NUNEZ 28040 MADRID SPAIN
1	CARLOS III UNIV OF MADRID ATTN C NAVARRO ESCUELA POLITEENICA SUPERIOR C/. BUTARQUE 15 28911 LEGANES MADRID SPAIN
1	UNIVERSIDAD DE OVIEDO FACULTAD DE QUIMICA DEPARTAMENTO DE QUIMICA FISICA Y ANALITICA ATTN E FRANCISCO AVENIDA JULIAN CLAVERIA S/N 33006 - OVIEDO SPAIN

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	DYNAMIC RESEARCH AB ATTN AKE PERSSON PARADISGRAND 7 SODERTALJE S 151 36 SWEDEN
3	NATL DEFENCE RESEARCH EST ATTN LARS HOLMBERG ULF LINDEBERG LARS GUNNAR OLSSON JOHAN FORSS FOA BOX 551 TUMBA S 14725 SWEDEN
2	SWEDISH DEFENCE RSCH ESTAB DIVISION OF MATERIALS ATTN S J SAVAGE J ERIKSON S17290 STOCKHOLM SWEDEN
3	SWEDISH DEFENCE RSCH ESTAB ATTN L HOLMBERG B JANZON I MELLGARD BOX 551 S14725 TUMBA SWEDEN
1	K&W THUN ATTN W LANZ ALLMENDSSTRASSE 86 CH 3602 THUN SWITZERLAND
2	AWE ATTN MICHAEL GERMAN WAYNE HARRISON FOULNESS ESSEX SS3 9XE UNITED KINGDOM
1	CENTURY DYNAMICS LTD ATTN NIGEL FRANCIS DYNAMICS HOUSE HURST RD HORSHAM WEST SUSSEX RH12 2DT UNITED KINGDOM

NO. OF
COPIES ORGANIZATION

- 6 DEFENCE RESEARCH AGENCY
ATTN W A J CARSON
I CROUCH
C FREW
T HAWKINS
B JAMES
B SHRUBSALL
CHOBHAM LANE CHERTSEY
SURREY KT16 0EE
UNITED KINGDOM
- 1 ROYAL ARMAMENT R&D ESTAB
ATTN I CULLIS
FORT HALSTEAD
SEVENOAKS KENT TN14 7BJ
UNITED KINGDOM
- 1 UK MINISTRY OF DEFENCE
ATTN GRAHAM J CAMBRAY
CBDE PORTON DOWN SALISBURY
WILTSHIRE SPR 0JQ
UNITED KINGDOM
- 2 UNIVERSITY OF KENT
UNIT FOR SPACE SCIENCES
ATTN PHILIPPE GENTA
PAUL RATCLIFF
CANTERBURY KENT CT2 7NR
UNITED KINGDOM
- 7 INSTITUTE FOR PROBLEMS IN
MATERIALS STRENGTH
ATTN S FIRSTOV
B GALANOV
O GRIGORIEV
V KARTUZOV
V KOVTUN
Y MILMAN
V TREFILOV
3, KRHYZHANOVSKY STR
252142, KIEV-142
UKRAINE
- 1 INSTITUTE FOR PROBLEMS OF STRENGTH
ATTN G STEPANOV
TIMIRYAZEVSKEY STR 2
252014 KIEV
UKRAINE

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
<small>Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</small>				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE March 1997	3. REPORT TYPE AND DATES COVERED Final, Jan - Mar 97		
4. TITLE AND SUBTITLE Elastic Behavior of an Atomic Lattice Under Large Volumetric Strains: The Quasi-Harmonic Idealization		5. FUNDING NUMBERS 61102AH43		
6. AUTHOR(S) Steven B. Segletes				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory ATTN: AMSRL-WM-TD Aberdeen Proving Ground, MD 21005-5066		8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-1357		
9. SPONSORING/MONITORING AGENCY NAMES(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING AGENCY REPORT NUMBER		
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.		12b. DISTRIBUTION CODE		
13. ABSTRACT (Maximum 200 words) <p>The implications of Segletes' recent equation of state are examined, when idealized to the condition defined as quasi-harmonicity. Results indicate that at large volumetric strains, a proportionality no longer holds, in general, between the volumetric and vibrational stiffnesses. The governing relation between these two stiffnesses is presented and is a function of the characteristic frequency of the lattice, alternately expressed in terms of the lattice spacing. It is further shown that the quasi-harmonic idealization of Segletes' equation will approach the harmonic approximation in the limit.</p>				
14. SUBJECT TERMS harmonic, lattice, vibration, equation of state, frequency		15. NUMBER OF PAGES 49		
		16. PRICE CODE		
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

INTENTIONALLY LEFT BLANK.

USER EVALUATION SHEET/CHANGE OF ADDRESS

This Laboratory undertakes a continuing effort to improve the quality of the reports it publishes. Your comments/answers to the items/questions below will aid us in our efforts.

1. ARL Report Number/Author ARL-TR-1357 (Segletes) Date of Report May 1997

2. Date Report Received _____

3. Does this report satisfy a need? (Comment on purpose, related project, or other area of interest for which the report will be used.) _____

4. Specifically, how is the report being used? (Information source, design data, procedure, source of ideas, etc.) _____

5. Has the information in this report led to any quantitative savings as far as man-hours or dollars saved, operating costs avoided, or efficiencies achieved, etc? If so, please elaborate. _____

6. General Comments. What do you think should be changed to improve future reports? (Indicate changes to organization, technical content, format, etc.) _____

CURRENT
ADDRESS

Organization

Name

E-mail Name

Street or P.O. Box No.

City, State, Zip Code

7. If indicating a Change of Address or Address Correction, please provide the Current or Correct address above and the Old or Incorrect address below.

OLD
ADDRESS

Organization

Name

Street or P.O. Box No.

City, State, Zip Code

(Remove this sheet, fold as indicated, tape closed, and mail.)

(DO NOT STAPLE)

DEPARTMENT OF THE ARMY

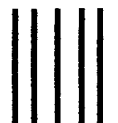
OFFICIAL BUSINESS

BUSINESS REPLY MAIL

FIRST CLASS PERMIT NO 0001,APG,MD

POSTAGE WILL BE PAID BY ADDRESSEE

DIRECTOR
US ARMY RESEARCH LABORATORY
ATTN AMSRL WM TD
ABERDEEN PROVING GROUND MD 21005-5066



NO POSTAGE
NECESSARY
IF MAILED
IN THE
UNITED STATES

